

MASSLESS FERMIONS IN EXTERNAL FIELDS IN TERMS OF HEUN'S FUNCTIONS

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In this paper, we integrate the (3+1)-dimensional Dirac equation for massless fermions, minimally coupled at static electric and magnetic external fields. For intense fields, the differential equation admits a closed-form analytical solution, expressed by biconfluent Heun functions (BHE). The obtained bi-spinors allow us to calculate the components of the four-current, and to obtain a special relation for the quantized energy as well. By cancelling out the electric field, the general relation of energy quantization finally leads to a discrete spectrum, similar to that obtained by Novoselov in graphene layers.

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1. Introduction

The revolutionary experimental results of the researchers K.S. Novoselov and A.K. Geim regarding the relativistic quantum effects of the Dirac fermions in graphene layers met a wide international interest, being true challenges in the theoretical and experimental studies developed in quantum mechanics [1, 2, 3].

The most recent experiments with graphene opened new ways in deep research of this wonder-material with his special structure of electronic layers. Due to its uncommon electronic spectrum, *having the zero width of the forbidden band and electronic states very close to zero energy*, the investigation of this semiconductor led to a new theory in the condensed matter physics. Some relativistic quantum phenomena can now be experimentally tested, even if some of them are not observable in high energy physics.

It is to be noticed that the conduction is performed by the tops of the cones, near the Dirac's points K and K' [4], closed to the margins of the Brillouin zone [5], due to the disappearance of the forbidden zone.

An important peculiarity is the extending the fully occupied band structure between these points, which leads to a linear dispersion relation ($E = \pm \hbar |k| \nu_F$) as a proof for the existence of the massless relativistic particles. The experiments showed that the charge carriers are precisely the massless Dirac fermions [6], so that the low-energy electronic states between the above mentioned points can be described by the help of Dirac equation.

The effective “vacuum” medium offered by graphene helps to put into evidence both the relativistic quantum tunneling described by the Klein paradox, and some other relevant phenomena offered by quantum electrodynamics [7]. Consequently, the penetration of relativistic particles through large potential barriers can be experimentally tested using this material [8].

Experimental realization of the quantum Hall effect in graphene at the room temperature [9] is explained by the fact that the transmission diminishes with the increase of the potential barrier, while the discrete energetic states of the positrons inside the barrier get aligned with the continuous energetic states of the electrons outside the barrier. The mixture of the wave functions of electrons and positrons lead to a high tunneling probability, as described by the Klein paradox [8].

It is important to mention that the wave functions corresponding to the quantum states of different physical systems (*e.g.* the isotropic harmonic oscillator, the three-dimensional oscillator, and the double anharmonic oscillator) lead to Heun polynomials, having a nice behavior at the singular points [10]. The advantage of these functions is that they help to obtain exact solutions in theoretical estimations of some macroscopic quantities. The polynomial solutions of the Heun equation are specially important and have been analyzed by different authors [11, 12, 13].

The aforementioned papers show the importance of the Heun equation and its wide possibility of investigation.

This paper generalizes the results recently obtained by the author [14] concerning the biconfluent Heun equation, as being satisfied by the spinor ξ and φ components in an intense electric field [15]. The wave function, the general relation of the quantized energy, and the dependence of the currents and charge density on the external fields are also obtained.

2. The Dirac-type equation

Following the same idea as in paper [14], we start with the (3+1)-dimensional Dirac equation written for the massless fermions, minimally coupled in the electric and magnetic external fields

$$\gamma^i D_i \Psi = 0, \quad (1)$$

where D_i is the gauge covariant derivative,

$$D_i = \partial_i - iq A_i, \tag{2}$$

with the four-potential $A_{i=\overline{1,4}}$ corresponding to orthogonal electric and magnetic fields $\mathbf{E}_0, \mathbf{B}_0$, oriented along Ox and Oz axes

$$A_2 = B_0 x; \quad A_4 = E_0 x. \tag{3}$$

We shall use the natural unit system $\hbar = c = 1$ and make allowance for the von Neumann matrices

$$\gamma^\mu = -i\beta\alpha^\mu; \quad \gamma^4 = -i\beta. \tag{4}$$

Here we used the Dirac representation

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}; \quad \alpha^\mu = \begin{pmatrix} 0 & \sigma^\mu \\ \sigma^\mu & 0 \end{pmatrix},$$

where σ^μ are the Pauli matrices.

We look for a solution of the Dirac equation

$$\gamma^\mu(\partial_\mu - iqA_\mu)\Psi + \gamma^4(\partial_4 - iqA_4)\Psi = 0 \tag{5}$$

of the form

$$\Psi(x, y, z, t) = e^{i(p_y y + k z - w t)} \begin{pmatrix} \xi(x) \\ \varphi(x) \end{pmatrix}, \tag{6}$$

where w is the energy of the chiral fermions.

For the spinors with two components ξ and φ , the Dirac equation yields the system

$$\begin{aligned} \sigma^1 \xi' + i\sigma^2(p_y - qB_0 x)\xi + i\sigma^3 k \xi &= i(w + qE_0 x)\varphi, \\ \sigma^1 \varphi' + i\sigma^2(p_y - qB_0 x)\varphi + i\sigma^3 k \varphi &= i(w + qE_0 x)\xi, \end{aligned} \tag{7}$$

where “'” stands for the derivative with respect to x .

Using the usual procedure, we write $\varphi(x)$ given by the first equation of the system (7)

$$\varphi = -\frac{i}{(w + qE_0 x)} \left[\sigma^1 \xi' + i\sigma^2(p_y - qB_0 x)\xi + i\sigma^3 k \xi \right] \tag{8}$$

take its derivative, and introduce the result into the second equation (7). Then we are left with

$$\begin{aligned} \xi'' - \frac{qE_0}{w + qE_0 x} \xi' - \frac{iq}{w + qE_0 x} \left[(wB_0 + p_y E_0)\sigma^1 \sigma^2 + E_0 k \sigma^1 \sigma^3 \right] \xi \\ = \left[- (w + qE_0 x)^2 + (p_y - qB_0 x)^2 + k^2 \right] \xi. \end{aligned} \tag{9}$$

3. Massless particles in static fields

Due to its complicated form, equation (9) has been approached by a first-order perturbative method in paper [14]. If the electric and magnetic fields are intense, this formalism is not applicable anymore and we proceed to solve the equation (9) which, for $k = 0$, becomes

$$\begin{aligned} \xi'' - \frac{qE_0}{w + qE_0x} \xi' - \frac{iq}{\hbar(w + qE_0x)} [(wB_0 + p_y E_0) \sigma^1 \sigma^2] \xi \\ = \left[-\frac{(w + qE_0x)^2}{c^2 \hbar^2} + \frac{1}{\hbar^2} (p_y - qB_0x)^2 \right] \xi, \end{aligned} \quad (10)$$

where we have reintroduced numerical values of the constants c and \hbar , in order to estimate the eventual numerical values of the obtained quantities. The spinor ξ writes as a one-column matrix

$$\xi = \begin{pmatrix} \xi_1(x) \\ \xi_2(x) \end{pmatrix}.$$

Introducing the new variable

$$x_* = x + \frac{w}{qE_0} \quad (11)$$

as well as the parameters

$$p = p_y + w \frac{B_0}{E_0}; \quad b = qB_0; \quad d = qE_0, \quad (12)$$

equation (10) leads to

$$\frac{d^2 \xi_{1,2}}{dx_*^2} - \frac{1}{x_*} \frac{d\xi_{1,2}}{dx_*} + \frac{\epsilon p}{\hbar x_*} \xi_{1,2} + \frac{1}{\hbar^2 c^2} \left[d^2 x_*^2 - b^2 c^2 \left(x_* - \frac{p}{b} \right)^2 \right] \xi_{1,2} = 0 \quad (13)$$

with $\epsilon = \pm 1$

We now perform the change of variable

$$\xi(x_*) = x_*^2 \exp [a_1 x_*^2 + b_1 x_*] y(x_*), \quad (14)$$

where

$$a_1 = \pm \frac{\sqrt{b^2 c^2 - d^2}}{2\hbar c}; \quad b_1 = -\frac{bp}{2a_1 \hbar^2} = \mp \frac{bpc}{\hbar \sqrt{b^2 c^2 - d^2}}, \quad (15)$$

and the condition $bc > d$ has been assumed. Equation (13) then becomes

$$\frac{d^2y}{dx_*^2} + \frac{4a_1x_*^2 - \frac{bp}{a_1\hbar^2}x_* + 3}{x_*} \frac{dy}{dx} + \left\{ \left[\frac{p^2}{\hbar^2} \left(\frac{b^2}{4\hbar^2 a_1^2} - 1 \right) + 8a_1 \right] x_* + \frac{p}{\hbar} \left[\epsilon - \frac{3}{2} \frac{b}{a_1\hbar} \right] \right\} \frac{y}{x_*} = 0, \quad (16)$$

or, with the new change of variable $x_* = \lambda z$,

$$\frac{d^2y}{dz^2} + \frac{4a_1\lambda^2z^2 - \frac{bp}{a_1\hbar^2}\lambda z + 3}{z} \frac{dy}{dz} + \left\{ \left[\frac{p^2}{\hbar^2} \left(\frac{b^2}{4\hbar^2 a_1^2} - 1 \right) + 8a_1 \right] \lambda^2 z + \frac{p\lambda}{\hbar} \left(\epsilon - \frac{3}{2} \frac{b}{a_1\hbar} \right) \right\} \frac{y}{z} = 0. \quad (17)$$

This equation can be written as

$$\frac{d^2y}{dz^2} + \frac{-2z^2 - \beta z + \alpha + 1}{z} \frac{dy}{dz} + \left[(\gamma - \alpha - 2)z - \frac{\delta + \beta + \beta\alpha}{2} \right] \frac{y}{z} = 0 \quad (18)$$

with standard initial conditions [15]

$$y(0) = 1; \quad y'(0) = \frac{\delta + \beta\alpha + \beta}{2\alpha + 2}.$$

The solution of equation (17) is, therefore, the function HeunB $(\alpha, \beta, \gamma, \delta, z)$ [16], where

$$\begin{aligned} a_1 &= \pm \frac{1}{2\hbar c} \sqrt{b^2 c^2 - d^2} = -\frac{1}{2\lambda^2}; & b_1 &= \frac{bp\lambda^2}{\hbar^2}; & \alpha &= 2; \\ \beta &= -\frac{2bp\lambda^3}{\hbar^2}; & \gamma &= \frac{p^2\lambda^2}{\hbar^2} \left(\frac{b^2\lambda^4}{\hbar^2} - 1 \right) = \frac{p^2 d^2 \lambda^6}{\hbar^4 c^2}; & \delta &= \mp \frac{2p\lambda}{\hbar}. \end{aligned} \quad (19)$$

The behavior of the wave function, and, consequently, of the spinor ξ is dictated by the exponential function $e^{a_1x_*^2 + b_1x_*}$. If the coefficient a_1 is positive, the solution goes to infinity. This fact determines us to take $a_1 < 0$.

The solutions of the equation (13), in their final form, therefore are

$$\xi_1 = \left(\frac{x_*}{\lambda} \right)^2 \exp \left[-\frac{x_*^2}{2\lambda^2} + \frac{bp\lambda^2}{\hbar^2} x_* \right] \text{HeunB} \left(2, -\frac{2bp\lambda^3}{\hbar^2}, \frac{p^2 d^2 \lambda^6}{\hbar^4 c^2}, -\frac{2p\lambda}{\hbar}; \frac{x_*}{\lambda} \right), \quad (20)$$

$$\xi_2 = \left(\frac{x_*}{\lambda} \right)^2 \exp \left[-\frac{x_*^2}{2\lambda^2} + \frac{bp\lambda^2}{\hbar^2} x_* \right] \text{HeunB} \left(2, -\frac{2bp\lambda^3}{\hbar^2}, \frac{p^2 d^2 \lambda^6}{\hbar^4 c^2}, \frac{2p\lambda}{\hbar}; \frac{x_*}{\lambda} \right). \quad (21)$$

The components of the other spinor satisfy an equation of the same type which, in our case, is identical with (13), that is

$$\frac{d^2\varphi_{1,2}}{dx_*^2} - \frac{1}{x_*} \frac{d\varphi_{1,2}}{dx_*} + \frac{\epsilon p}{\hbar x_*} \varphi_{1,2} + \frac{1}{\hbar^2 c^2} \left[d^2 x_*^2 - b^2 c^2 \left(x_* - \frac{p}{b} \right)^2 \right] \varphi_{1,2} = 0.$$

The solutions of the two equations are connected by the following functional algebraic equations of mixed type

$$\begin{aligned} \varphi_1(x_*) &= -\frac{ic/d}{x_*} \left[\hbar \frac{d\xi_2}{dx_*} - b \left(x_* - \frac{p}{b} \right) \xi_2 \right], \\ \varphi_2(x_*) &= -\frac{ic/d}{x_*} \left[\hbar \frac{d\xi_1}{dx_*} + b \left(x_* - \frac{p}{b} \right) \xi_1 \right]. \end{aligned} \tag{22}$$

4. The conserved current density components

The results obtained so far allow us to calculate the components of the four-current, by means of the general relations

$$\begin{aligned} j_\mu^n &= q\Psi^+ \alpha_\mu \Psi, \\ \rho_e^n &= q\Psi^+ \Psi = q \left[|\varphi_1|^2 + |\varphi_2|^2 + \xi_1^2 + \xi_2^2 \right], \end{aligned}$$

where $n = 0, 1, 2, \dots$. Since ξ_1 and ξ_2 are real, while φ_1 and φ_2 are purely imaginary, the only non-zero component is j_y , that is

$$\begin{aligned} j_y &= q\Psi^+ \alpha^2 \Psi = 2iq(\varphi_2 \xi_1 - \varphi_1 \xi_2) \\ &= \frac{2cq}{dx_*} \left[\hbar \left(\xi_1 \frac{d\xi_1}{dx_*} - \xi_2 \frac{d\xi_2}{dx_*} \right) + b \left(x_* - \frac{p}{b} \right) (\xi_1^2 + \xi_2^2) \right]. \end{aligned} \tag{23}$$

We now impose the condition that the parameters α and γ are related by

$$\gamma = 2(n + 1) + \alpha; \quad n = 0, 1, 2, \dots \tag{24}$$

which leads to

$$\frac{p^2 d^2 \lambda^6}{\hbar^4 c^2} = 2(n + 2),$$

or, if we use (12) and (19),

$$w = -\frac{E_0}{B_0} p_y + c \sqrt{2(n + 2) \hbar q B_0} \left[1 - \left(\frac{E_0}{c B_0} \right)^2 \right]^{3/4}, \tag{25}$$

which is the final expression for the quantized energy. As one observes, if the electric field vanishes, the last formula yields the energetic discrete spectrum obtained by Novoselov in graphene layer [6]

$$w_{E=0} = \nu_F \sqrt{2(n+2)\hbar q B_0}.$$

Recently, in addition to the above mentioned integer and the fractional quantum Hall effect, Novoselov has observed relativistic effects [6] in graphene samples whose crystalline structure has two atoms per unit cell. In this case, there exists a linear energy-momentum relation for electrons $w = p v_F$, which in the presence of a magnetic field becomes

$$w = \pm \sqrt{2q B_0 \hbar v_F^2 \left(\nu + \frac{1}{2} \pm \frac{1}{2}\right)}; \quad \nu = 0, 1, 2, \dots$$

being connected to chirality by the term $\pm 1/2$.

5. Conclusion

Using the (3+1)-dimensional Dirac equation, we have described the behavior of massless fermions disposed in a system of mutually orthogonal electric and magnetic fields. In the presence of an intense electric field, and of a magnetic field orthogonal to the sample plane, the differential equation admits a closed-form analytical solution, the components of the spinors ξ and φ satisfying the biconfluent Heun differential equation [16]. The wave function, the dependence of the currents and charge density on the external fields, as well as the general quantized expression for energy are also obtained. If the electric field vanishes, our result becomes similar to that obtained by Novoselov in graphene layers.

There exists a number of experimental and theoretical investigations on this subject [17, 18, 19], but we feel that our theoretical results are more general. We also mention, as a new result, the expression for spinor components in closed analytical form, in terms of the functions HeunB, rediscovered and widely applied in physics and chemistry.

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